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ABSTRACT

Materials properties measurements are made for the RDX-based explosive, PBXN-109, and an initial ALE3D model for cookoff is discussed. A significant effort is underway in the U.S. Navy and Department of Energy (DOE) laboratories to understand the thermal explosion behavior of this material. Benchmark cookoff experiments are being performed by the U.S. Navy to validate DOE materials models and computer codes. The ALE3D computer code can model the coupled thermal, mechanical, and chemical behavior of heating and ignition in cookoff tests. In order to provide a predictive capability, materials characterization measurements are being performed to specify parameters in these models. We report on progress in the development of these ALE3D materials models and present measurements as a function of temperature for thermal expansion, heat capacity, shear modulus, bulk modulus, and One-Dimensional-Time-to-Explosion (ODTX).

INTRODUCTION

Computational tools are being developed to predict the response of Navy ordnance to abnormal thermal (cookoff) events. The Naval Air Warfare Center[1] (NAWC) and Naval Surface Warfare Center (NSWC) are performing cookoff experiments to help validate DOE computer codes and associated thermal, chemical, and mechanical models. Initial work at the NAWC is focused on the cookoff of an aluminized, RDX-based explosive, PBXN-109 that is initially confined in a tube with sealed ends (see Figure 1). The tube is slowly heated until ignition occurs. The response is characterized using thermocouples, strain gauges, and high-speed cameras. A modified version of this system is being developed at the NSWC. The designs of these cookoff systems are relatively simple to facilitate initial model development. An effort is being made to achieve a wide range of results for reaction violence.

Lawrence Livermore National Laboratories (LLNL) and Sandia National Laboratories (SNL) are developing computer codes and materials models to simulate cookoff for ordnance safety evaluations. The computer program ALE3D from LLNL is being used to simulate the coupled thermal transport, chemical reactions, and mechanical response during heating and explosion[2]. SNL is employing multiple computer codes in a parallel effort[3,4,5]. For the analysis of PBXN-109 cookoff, Schmitt et al.[6] performed an initial survey of measured materials properties and provided estimates for several others. In addition, they performed initial predictions of the time to explosion for a small-scale NSWC cookoff system. In this paper, we report on the development of ALE3D models for cookoff of PBXN-109 in the NAWC system of Figure 1. In addition, measurements are given for thermal expansion, heat capacity, shear modulus, bulk modulus, and ODTX.

MODEL VALIDATION EXPERIMENTS

The NAWC is performing cookoff tests with cylindrical charges of PBXN-109 confined in a steel tube with sealed ends[1] (see Figure 1). The explosive has a nominal aspect ratio of L/D=4, and a diameter nearly matching the inside diameter of the tube. For a representative test (No. 000407) the tube has a 2.54 cm outer diameter with a 0.89 mm wall thickness providing a confinement pressure of approximately 0.4 kbar (40 MPa). The end seals are achieved with torque-n-seal plugs secured with retaining rings. Ullage is adjusted at the ends of the energetic material by changing the axial positions of the end plugs. Insulating materials are placed at the ends of the explosive and tube. An insulated wire wrap provides the energy to heat the tube. The assembly is mounted horizontally in a vise and enclosed in a sealed box.

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The temperature is measured at seven locations on the outer tube surface using thermocouples. A Proportional-Integral-Derivative controller is used to adjust the heater power to

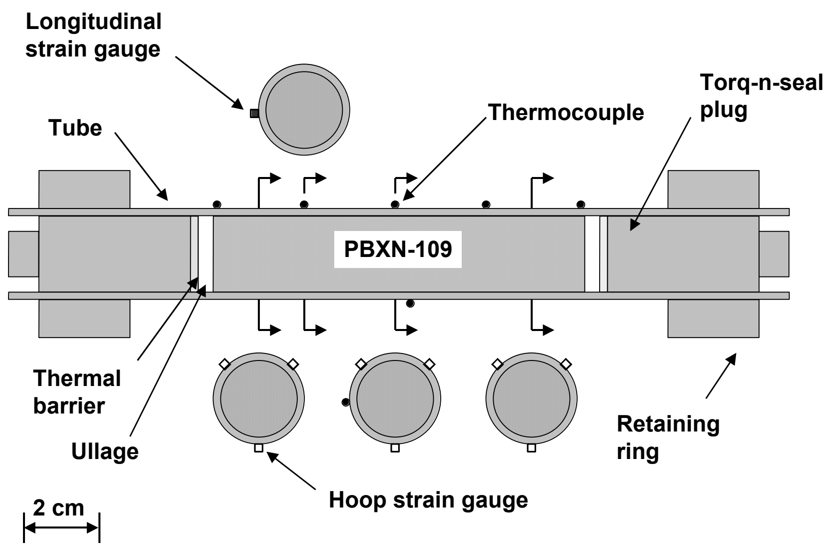

Figure 1 Schematic of geometry and instrumentation for NAWC cookoff in Test No. 000407.

keep the center-top temperature near the set-point value. Nine hoop strain gauges and one longitudinal strain gauge are used to measure the deformation of the tube during thermal ramp and explosion. A high-speed camera is available to monitor the expansion and fragmentation of the assembly.

In experiments performed to date, the set-point tube temperature has been ramped quickly to 130°C and then ramped at 6°C/h until ignition occurs. Measured temperature profiles in Test No. 000407 are shown in Figure 2a. The center-top temperature is 176°C at ignition. The far right and far left temperatures at the tube are approximately 20°C cooler at this same time, indicating a significant temperature gradient along the tube. This temperature profile assures that ignition occurs at a location midway between the axial ends as confirmed by the fragments in Figure 2b. In addition, the tube fragments are relatively large indicating mild violence. It is possible that a more uniform temperature profile would yield more violence. In other tests, the tube wall thickness and ullage at the ends of the HE have been varied.

ALE3D MODEL

ALE3D chemical, mechanical, and thermal models are being developed to model the cookoff of PBXN-109. In our initial model, the chemical reaction sequence is taken to have four components with three reaction steps following the model developed by McGuire and Tarver[7] for pure RDX:

$$A \rightarrow B \qquad r_1 = Z_1 \exp(-E_1/RT)\rho_A \qquad (1)$$

$$B \rightarrow C \qquad r_2 = Z_2 \exp(-E_2/RT)\rho_B \qquad (2)$$

$$C \rightarrow D \qquad r_3 = Z_3 \exp(-E_3/RT)\rho_C^2 \qquad (3)$$

Here ρ_i is the mass concentration of a reactant i. The quantities r_j, Z_j and E_j are the reaction rate, frequency factor and activation energy, respectively, for a reaction j. Component A is the starting material including RDX, aluminum, and binder. Component B is also a solid intermediate with material properties assumed to be the same as component A, and the components C and D are treated

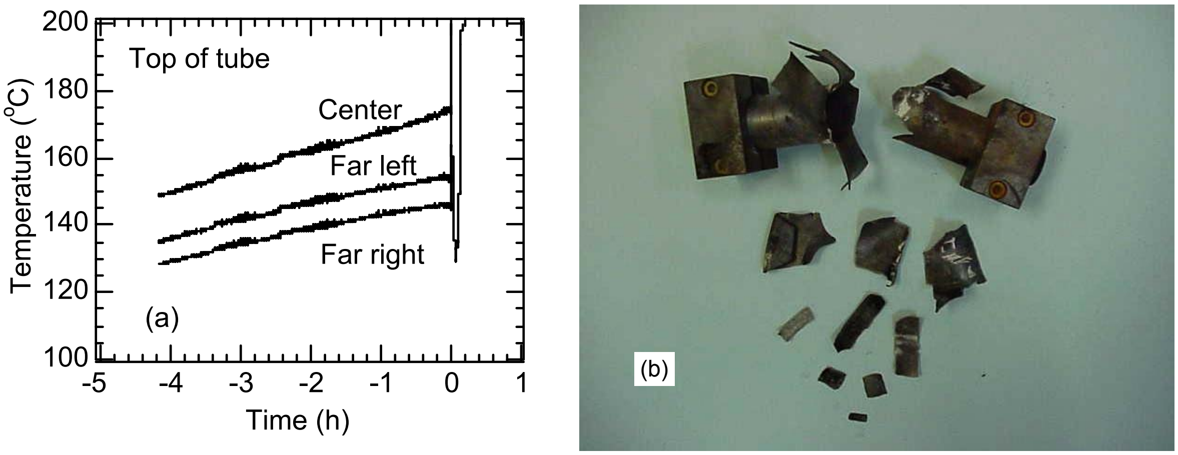

Figure 2 Results for Test No. 000407. (a) Thermocouple measurements. (b) Collected tube fragments.

as gases. The aluminum and binder are treated as inert until the last reaction step where they are converted to their final products. The selection of parameters and a comparison of model ODTX predictions with measured values is given below.

The time-dependent thermal transport model includes the temperature-dependent heat capacity and thermal conductivity. Thermal properties for materials A and B are assigned using the measurements of this project for PBXN-109. The temperature-dependent heat capacity for reactants C and D is assigned constant-volume values for the final product gases at a representative pressure of 1 kbar. They are calculated from the thermo-chemical equilibrium computer code, CHEETAH 2.0[8]. The thermal conductivity is estimated using Bridgman's[9] equation in which the sound velocity is calculated using results from CHEETAH.

The mechanical models for the model chemical constituents A and B along with the steel components are taken to have Steinberg-Guinan[10] strength models with polynomial expressions for the equations of state. The mixing rule of Reaugh and Lee[11] will be used to determine mixture parameters from those of the individual constituents. In addition, parameters for the starting material will be specified using the mechanical measurements of this project, including those described below. The model chemical components C and D are treated as no-strength materials with Gamma-Law equations of state. This equation of state is appropriate for the relatively low confinement pressures (~1 kbar) of these cookoff tests.

Boundary conditions are shown in Figure 3 for the cookoff setup of Test No. 000407 (see Figure 1). The model includes ullage on the side and ends of the explosive. Surfaces across the gap are considered to expand and slide without friction and to have negligible thermal contact resistance. The plug and retaining ring are assumed to be perfectly joined to the tube wall. The ends of the tube and plug at the spacer block are treated as free mechanical boundaries in which energy losses are handled with a heat transfer coefficient. The tube heater is modeled as a uniform thermal flux condition at the outside tube surface between the retaining rings. The heat flux is adjusted using a PID controller to maintain the top-center tube temperature at its set point value. Thermal convection and hemispherical radiation are present on the retaining ring surface and remaining outside surfaces of the tube.

The above ALE3D models will first be tested with one-dimensional and two-dimensional axisymmetric problems. Since all ALE3D calculations must currently be performed on 3D meshes, these calculations will be performed on meshes with the shape of thin wedges. This approach will greatly accelerate testing since calculations can be performed with far fewer nodes, variables, and computing time.

MATERIALS CHARACTERIZATION

<u>Sample specifications</u>

Chemical, mechanical, and thermal properties and parameters are needed for PBXN-109 to model the NAWC cookoff experiments. The PBXN-109 mixture has a nominal composition of 64% RDX,

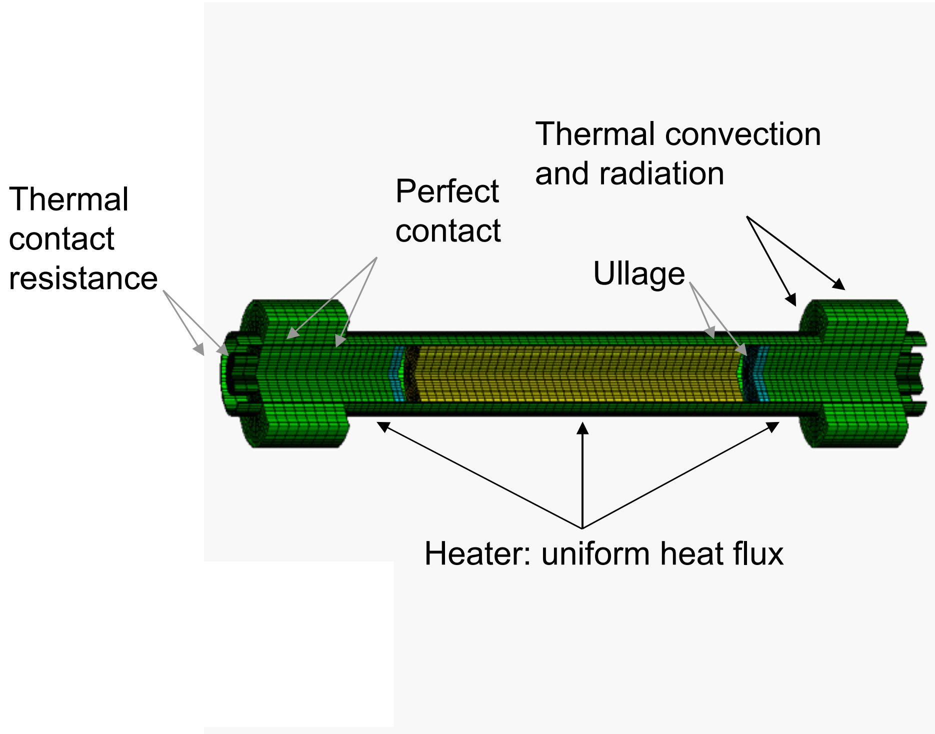

Figure 3 Mesh and boundary conditions for ALE3D model of NAWC cookoff Test No. 000407.

20% Al, and 16% HTPB/DOA binder by weight[12]. Here we report on measurements of Coefficient of Thermal Expansion (CTE), heat capacity, bulk modulus, shear modulus, and one-dimensional-time to explosion for PBXN-109. The samples were taken from mixture no. 991206 that is being used by the participants from LLNL, SNL, NAWC, and NSWC in this cookoff investigation. The density for this sample was measured by Paiz and Carey[13] to be 1.67 g/cm^3.

Coefficient of Thermal Expansion

Measurements of linear CTE were made for PBXN-109 using a Thermal Mechanical Analyzer (TMA) Model No. 2940 from TA Instruments. Calibration of the instrument was verified with an aluminum standard over the temperature range 25-114^{o}C. The measured aluminum value of 24.6 μm/m-^{o}C agrees well with the standard value of 24.8 μm/m-^{o}C. Measurements for PBXN-109 were made on 0.635 cm D x 0.635 cm L cylinders cut from larger samples. Variations in the sample dimensions and mounting were larger for this material than for a typical metal or explosive due to the rubber-like character of this material. Three tests for PBXN-109 yielded a CTE of 113$\pm$8 μm/m-^{o}C for a nominal temperature range of 25 to 115^{o}C (see Figure 4). Although the CTE is nearly constant over this range of temperatures, the small curvature may be lead to errors for large extrapolation. The primary contribution to measurement variation is believed to be the uncertainties in sample dimensions and alignment of the sample in the test fixtures. The measured CTE for PBXN-109 is in the general range of 100-200 μm/m-^{o}C for polymeric materials, and is considerably higher than the values of 25 and 64 μm/m-^{o}C for Al and RDX[14], respectively.

Heat Capacity

The heat capacity for PBXN-109 was made using a Differential Scanning Calorimeter (DSC) Model No. 2920 from TA Instruments[15]. The DSC measures the difference in the heat flow between a sample and an inert reference as the temperature of the stage is changed. The instrument was calibrated using a sapphire (Al_2O_3) standard and verified using a polystyrene (PS) standard. The 0.343 cm D x 0.0635 cm H sapphire standard was selected for the calibration since it could be used at the highest temperature of 140^{o}C for PBXN-109. In contrast, temperatures for the 0.474 cm D x 0.085 cm H

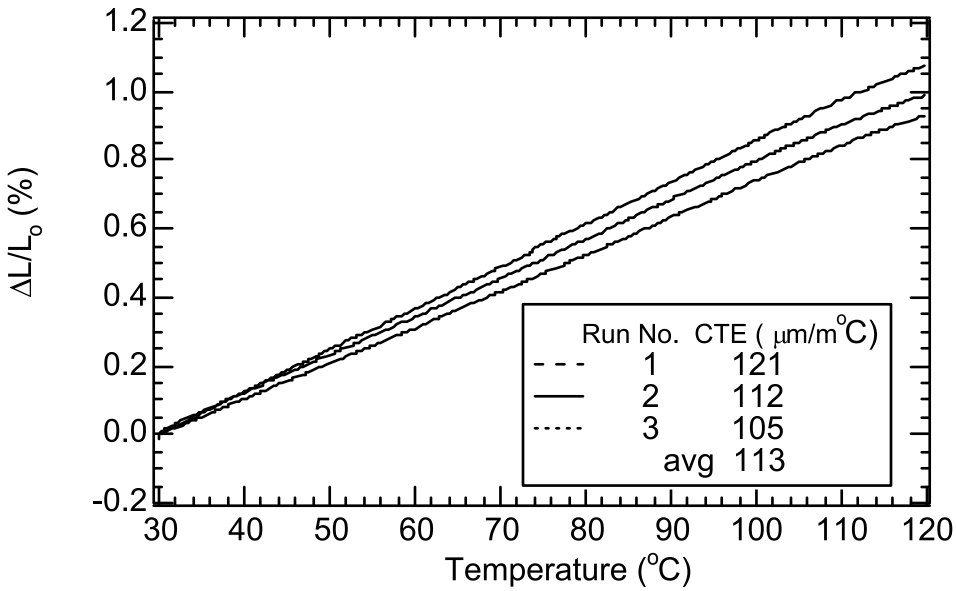

Figure 4 Measured thermal expansion of PBXN-109.

polystyrene sample are kept below 80^{o}C to avoid thermal alteration. The small thickness of each sample provides rapid thermal transport which minimizes thermal lag in the heating of the sample. All samples were encapsulated in aluminum pans, and a relatively high temperature ramp rate of 10^{o}C/min was selected for operation. Baselines were established using empty pans that were crimped together in the manner of the sample pans. Replicate measurements were performed for each standard. Measured values of the PS heat capacity agree with each other to within 1% for a given encapsulated sample. The averages of these measurements are within 1% of the standard values[16] (see Figure 5). The primary contributions to measurement error are believed to be variations in thermal contact resistance between the encapsulating aluminum pans, stage, and sample. Variations in encapsulation and crimping of the sample and reference pans have been observed to contribute several percent variations to the heat capacity results. This variation is much larger than the above-mentioned deviations of 1% associated

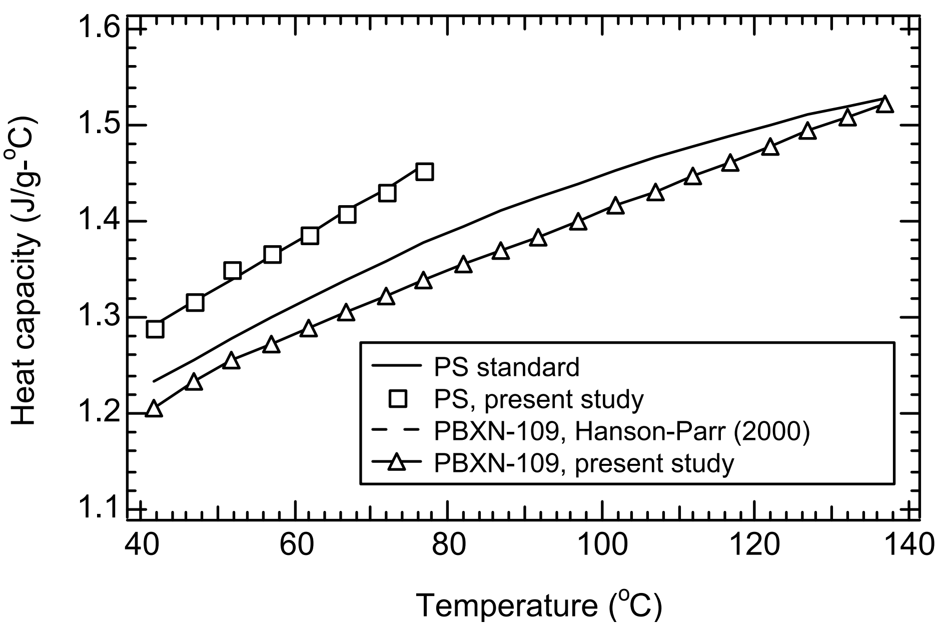

Figure 5 Comparsion of heat capacity measurements for polystyrene and PBXN-109.

with run-to-run variations with a single encapsulated sample. In addition, the lower thermal diffusivity for PS increases the thermal lag relative to sapphire. Finally, the rapid ramp rate amplifies these effects.

A 0.5 cm D x 0.1 cm H disk of PBXN-109 was fabricated and encapsulated in aluminum pans for heat capacity measurements. Measurements were made in two runs for this sample over the temperature range of 40-140^{o}C (see Figure 5). The results from the replicated runs agree with each other to within 1% and the averaged values agree with the curve-fit results from Hanson-Parr[17] to within 3%. For the Hanson-Parr data, the sample standard deviation is approximately 9%. At a given temperature, typically 6 measurements were made to give a standard deviation of the mean $\sigma/n^{1/2}$=4%. Thus, the measurements of the two studies agree within measurement uncertainty. In addition to the factors mentioned above, irregularities in the sample shape from cutting may have added to thermal contact resistance and measurement error.

Shear Modulus

The shear storage and loss moduli were measured for PBXN-109 as a function of strain rate and temperature using a Rheometrics Mechanical Spectrometer. Rectangular samples 3.18 x 1.27 x 0.318 cm were cut for testing. Three room temperature tests were performed at a frequency of 1 cycle/s. In each test, the strain was increased from 0 to 1.8%, which increased the shear rate from 0 to 0.11 s^{-1} (see Figure 6). The average shear storage modulus decreases approximately 26% as the shear strain and rate increases (see Figure 6). The standard deviation for the storage modulus is approximately 13% for the three runs. The loss modulus is approximately a factor of five less than the storage modulus. Measurements for the shear storage and loss moduli were made at 1 cycle/s over the temperature range 25 to 120^{o}C. The storage and loss moduli decrease by approximately 25 and 75%, respectively as the temperature is increased (see Figure 7). The primary contributions to measurement error are irregularities in the sample geometry and alignment of the sample in the test fixtures.

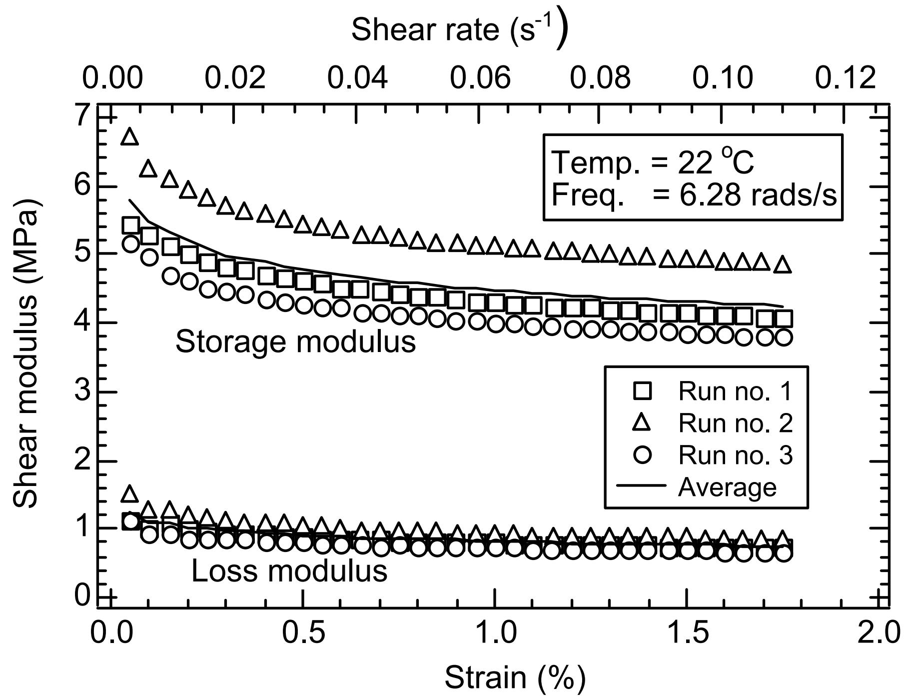

Figure 6 Measured shear modulus versus strain at for PBXN-109 at 1 cycle/s and room temperature.

Bulk Modulus

The bulk modulus was measured by means of a confined compression test[18,19]. The hydraulic piston of an MTS machine was used to uniaxially compress a 1.27 cm D x 2.54 cm L sample in a cylindrical die of the same diameter. In each test, the displacement of the piston was measured while the load was increased at a constant rate. Corrections were made in the displacement data for deflection of the test fixtures. This method was selected since it can provide good results for rubber-like materials in which the shear modulus is small compared to the elastic modulus[18,19] (Poisson's ratio~0.5). In this situation, the compressive loading is nearly hydrostatic.

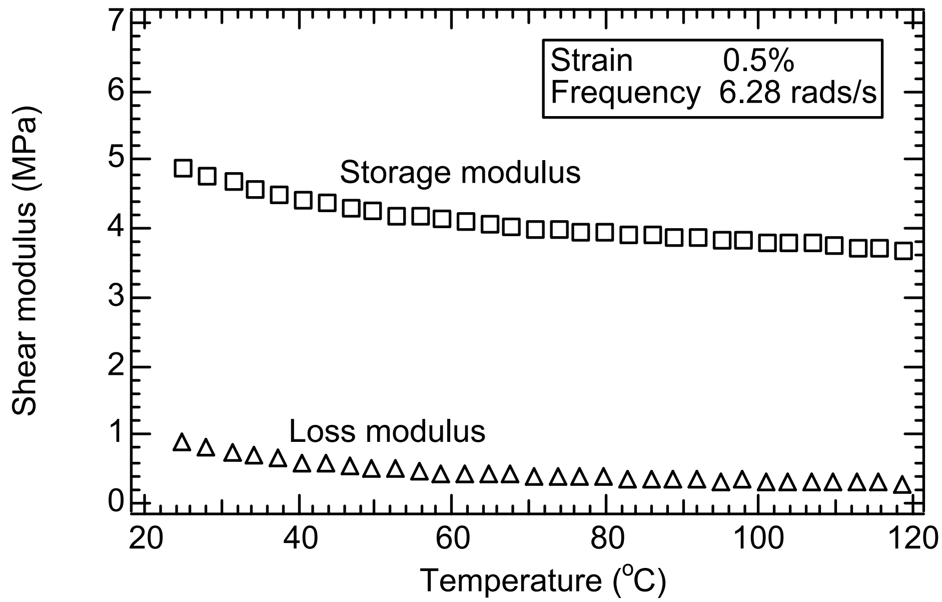

Figure 7 Measured shear moduli versus temperature for PBXN-109 at 1 cycle/s and 0.5% strain.

In order to verify the method, bulk modulus measurements were made for Silastic J, a well-characterized rubber. At room temperature, the compressive stress was increased from 0 to 31.0 MPa at a rate of 0.690 MPa/s. The measured compressive stress for Silastic J is plotted versus volumetric strain in Figure 8. These results compare quite favorably to the measurements of DeTeresa[20]. The latter

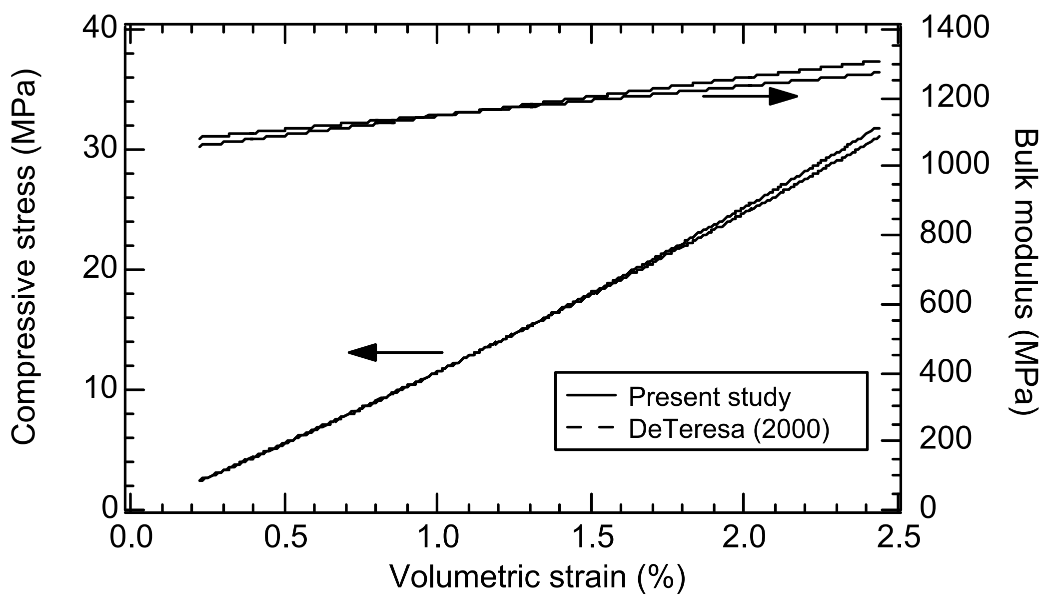

Figure 8 Measured compressive stress and bulk modulus versus volumetric strain for Silastic J at T=22°C.

measurements were obtained by compressing an immersed sample to provide true hydrostatic compression. Strain-dependent expressions for the bulk modulus are obtained for the two sets of results using

$$K = d\sigma/d\varepsilon_v \qquad (4)$$

Here K is the bulk modulus, σ is the compressive stress, and ε_v is the volumetric strain. The resulting curves show a 20% increase in bulk modulus for Silastic J. In addition, there is excellent agreement between the present results and those of DeTeresa[20] (see Figure 8), verifying the correction operation of the apparatus.

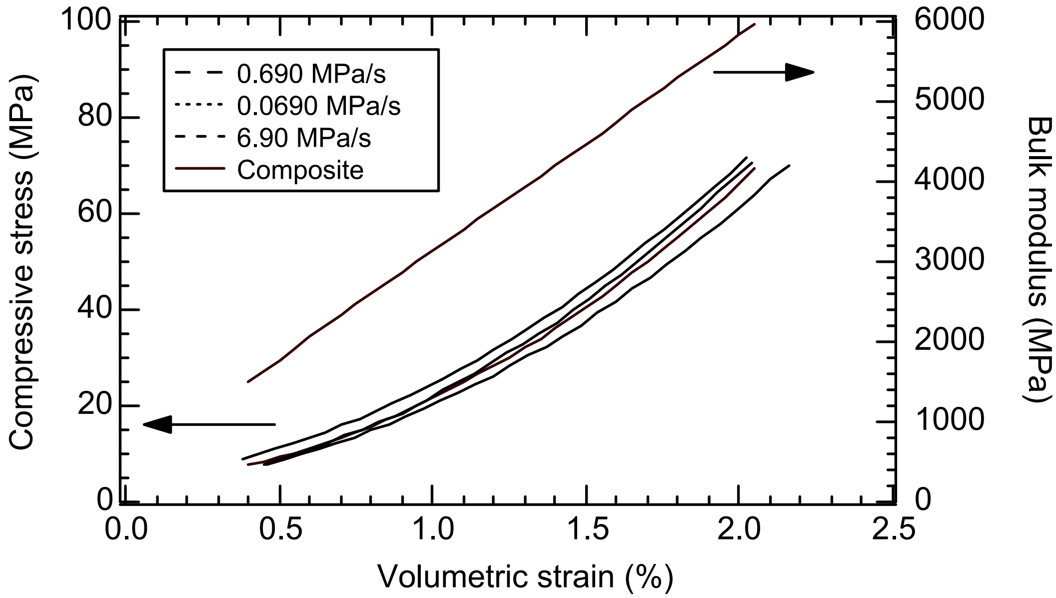

Figure 9 Measured compressive stress and bulk modulus versus volumetric strain for PBXN-109 at T=22^{o}C.

Bulk modulus measurements were performed for a single sample of PBXN-109 at room temperature and loads ramped to 69.0 MPa. Three tests were performed for ramp rates of 0.690, 0.0690, and 6.90 MPa/ s (see Figure 9). These were the respective fourth, fifth, and sixth tests with this sample. In the three earlier tests, the sample was loaded to the same stress of 69.0 MPa at a temperature of 22^{o}C. The stress-strain curves are quite similar suggesting that ramp rate has little effect over the range of conditions considered. In addition, it does not appear that repeated mechanical cycling of this sample altered the mechanical properties of the sample in these three tests. However, there is still the possibility that changes to the sample could have occurred in the first three tests. A fitting procedure was performed to obtain a single composite stress-strain representing all three experimental curves. Application of Eq. (4) to this result gives the bulk modulus curve in Figure 9. It is seen that the bulk modulus varies by a factor of four over the range of strains, indicating that PBXN-109 provides relatively little resistance to compression at low strains and, but much more resistance at high strains.

There are several possible sources of experimental error for these measurements. The low modulus at low strains makes it difficult to determine the point of initial compression. In addition, irregularities in the sample geometry lead to uncertainties in the point at which the sample completely fills the die. Both of these factors contribute to an offset uncertainty in the volumetric strain. Finally, as mentioned above it is possible that the repeated load cycling could have altered the mechanical properties from those of the virgin material.

Estimates for Elastic_Modulus and Poisson's Ratio

Rough estimates for Poisson's ratio, ν and the elastic modulus, E, can be obtained using the following expressions with the observation that the measured bulk modulus is two to three orders of magnitude larger than the shear modulus[21], G (see Figures 7 and 9):

$$\nu = (3K - 2G)/(6K + 2G) \approx 0.5 \quad (2)$$

$$E = 2G(1 + \nu) \approx 3G \quad (3)$$

Here G is taken to be the storage modulus of Figure 7, and the results of Figure 9 are used for K. The rubber-like character of the material is confirmed with the estimated value of 0.5 for Poisson's ratio. This result also validates a key assumption of the test that the shear modulus is much less than the bulk modulus.

One-Dimensional-Time-to-Explosion

ODTX measurements were made using the standard apparatus at LLNL[22]. The central components of the ODTX apparatus are two identical cylindrical aluminum anvils, each containing a hemispherical sample cavity with a diameter of 1.27 cm and a knife-edge groove to accommodate a Cu gasket. A circular copper ring with 1.85 cm diameter is used to establish a gas-tight seal when the two anvils are pressed together. This provides an effective confinement area of 2.7 cm^2. The closing force is established by the hydraulic cylinder (effective area is 20.3 cm^2) pushing on the top anvil. The anvil confinement pressure can be set at 150 MPa by using a hydraulic pressure of 20 MPa (3000 psi). For unconfined tests, a 1 mm square groove was machined in one of the anvil surfaces providing a small opening when the anvils were pressed together. Preferential discharge of smoke from this opening indicated that the sample cavity was sufficiently exposed to ambient conditions.

PBXN-109 samples were hand carved into 0.5" (1.27 cm) diameter spheres. A 5/8" (1.59 cm) diameter cylinder is first cored from the bulk sample using a brass coring tool. Cylindrical pieces slightly longer than 1/2" in length were then sectioned out using a razor blade. Finally, a 1/2"-diameter scoop (similar to a mellon baller) was used to round off the pieces to produce the final spheres. The surface was also smoothed using the same tool. Sample weights are reproduced to within 10%.

In these experiments, the anvils were preheated to a pre-determined temperature. The anvils were briefly opened to allow delivery of a spherical explosive sample into the cavity. The anvils were then closed, and confinement was established by the hydraulic force. When the internal cavity pressure exceeds that of the closing force, the anvils pop apart with a loud report. The time to explosion is the elapsed time between the insertion of the spherical sample and the rupture of containment as registered by the microphone. A series of experiments were conducted with time to explosions ranging from 30 seconds to several hours.

The time to explosion for PBXN-109 as a function of temperature for samples under no confinement and heavy confinement (150 MPa) is shown in Figure 10. Results from earlier ODTX tests with PBXN-109 and RDX at 150 MPa confinement are also included for comparison. The confined and unconfined results of this study follow a single curve, indicating experimental reproducibility and the insensitivity of explosion time to pressure. These results are consistent with the earlier PBXN-109 results except at temperatures above 235^{o}C. In this temperature range the explosion times of this study show a much strong sensitivity to temperature. The scatter in the earlier PBXN-109 data is much larger at the higher temperatures and associated short explosion times of 1 to 10 s, suggesting an approach to the measurement limits of the apparatus. The earlier RDX explosion times are generally shorter than the PBXN-109 values. The thermal diffusivity of $3x10^{-3}$ cm^2/s for PBXN-109 is considerably higher than the RDX value of $5x10^{-4}$ cm^2/s which would tend to reduce hot spots in the PBXN-109 and make it less reactive relative to RDX. At lower temperatures and longer explosion times, the importance of thermal transport is reduced and behavior is governed by the reaction kinetics of RDX, leading to similar explosion times for RDX and PBXN-109. It is also worthwhile to note that the lowest explosion temperature of 175°C for PBXN-109 is quite close to the ignition temperature of 176°C in cookoff Test No. 000407 (see Figure 2a). Both tests involve long reaction times.

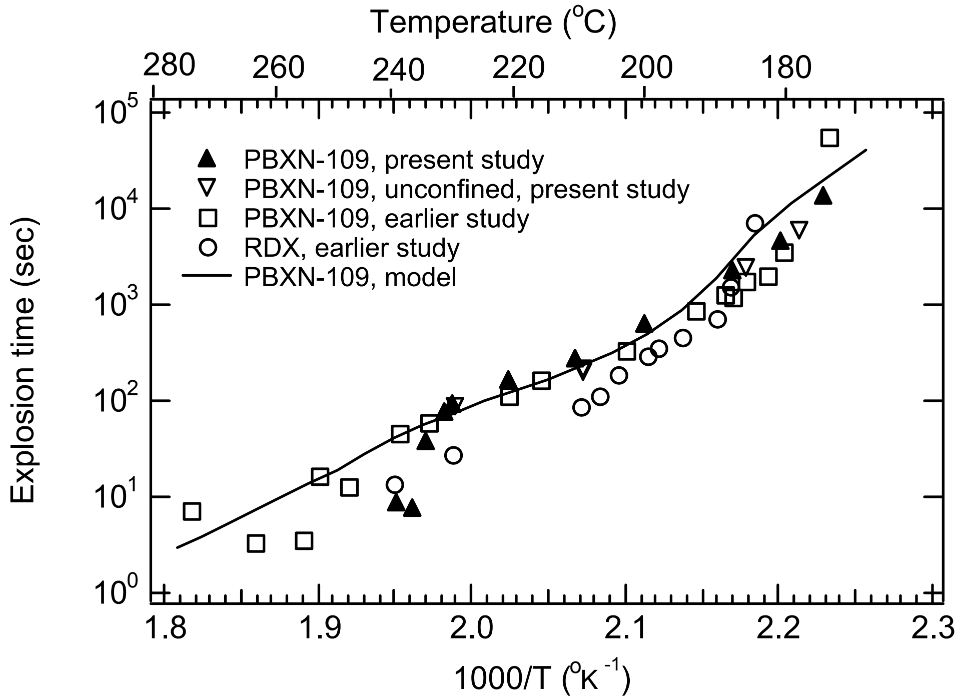

Figure 10 Comparison of ODTX results for PBXN-109 and RDX.

Calculated explosion times for PBXN-109 are also shown in Figure 10 for a one-dimensional model[7] involving transient heat conduction and the chemical reaction sequence (Eqs. (1)-(3)). In this model, the densities of each of the four components A, B, C, and D are taken to have the room temperature value of 1.67 g/cm^3. The two components A and B are assumed to have the same thermal transport properties. We use the heat capacity of this study (see Figure 5) and the thermal conductivity $\lambda=5.581\times10^{-3}+8.242\times10^{-6}T$ of Hanson-Parr[17] in which λ and T have the units of W/cm-°C and °C. The thermal properties for the gaseous products C and D are calculated using the strategy described in the above section on ALE3D modeling. The values Z_j and E_j of Table 1 are the same as those of McGuire and Tarver[7], except for Z_1 which is treated as an adjustable parameter. The earlier RDX heats of reaction q_1 and q_2 are reduced by 36% to account for the fraction of RDX present in

Table 1 Chemical Kinetics Parameters for PBXN-109

Reaction step	$\ln(Z_j)$	E_j kcal/g-mole-°K (kJ/g-mole-°K)	q_j cal/g (J/g)
A→B	41.0 s^{-1}	47.1 (197)	64 (268) endothermic
B→C	40.7 s^{-1}	44.1 (185)	-192 (-803) exothermic
C→D	34.49 s^{-1}-cm^3- g^{-1}	34.1 (143)	-1568 (-6560) exothermic

the mixture. Recall that aluminum and the binder are treated as inert until the final reaction step. The value for q_3 is calculated using q_1 and q_2 and the total heat of reaction of 1696 cal/g calculated from CHEETAH. One-dimensional explosion times were calculated using TOPAZ2D[23,24] and a mesh with 50 elements uniformly spaced in the radial direction. The time to explosion is taken to occur at the time that 10% of the initial mass of HE is converted to the final product D. The resulting model explosion times match the measured values over much of the temperature range (see Figure 10). However, there are larger discrepancies between the model values and the measurements of this study at temperatures above 235°C. Nonetheless, the model is expected to provide satisfactory results at the lower temperatures observed at ignition in the cookoff tests.

CONCLUSIONS

ALE3D chemical, mechanical, and thermal models are being developed to simulate the cookoff of PBXN-109 in NAWC and NSWC cookoff tests. In the NAWC cookoff experiments, a PBXN-109 sample with L/D=4, is heated slowly in a sealed tube until explosion. Thermocouple measurements and collected fragments for a representative test show ignition in the warm central region of the tube. Mild violence is indicated by the large size of the collected fragments. For the development of ALE3D models, a McGuire and Tarver[7] chemical kinetics model for RDX is applied to PBXN-109. A mesh is generated and boundary conditions are given for the NAWC cookoff test. The selection of parameters for strength models and equations of state is in progress. To help with the determination of these parameters, measurements are given for thermal expansion, heat capacity, shear modulus, bulk modulus, and one-dimensional time to explosion. These results are validated with standards, replicate measurements, and comparison with earlier results. The thermal expansion and moduli measurements reveal the rubber-like behavior of PBXN-109, resulting from the high binder content. The measured one-dimensional explosion times are generally longer than RDX values, and can be satisfactorily represented by a 1D thermal transport model with chemical kinetics.

ACKNOWLEDGMENTS

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NOMENCLATURE

DOA	Dioctyl adipate
DOE	Department of Energy
E	Elastic modulus, $M/(t^2L)$
E_j	Energy of activation for reaction j, E/(Tmole)
G	Shear modulus, $M/(t^2L)$
HTPB	Linear hydroxy-terminated polybutadiene
K	Bulk modulus, $M/(t^2L)$
n	Reaction order
NSWC	Naval Surface Warfare Center, Indian Head
ODTX	One-Dimensional Time to Explosion
PBXN-109	Aluminized RDX explosive
RDX	Cyclotrimethylene trinitramine
r_j	Rate of reaction j, $M/(L^3t)$
T	Temperature, T
Z_j	Frequency factor for reaction j, $L^{3(n-1)}/(M^{(n-1)}\ t)$
ε_v	Volumetric strain
λ	Thermal conductivity, E/(tLT)
ν	Poisson's ratio
ρ_i	Mass concentration of reactant i, M/L^3
σ	Compressive stress, $M/(t^2L)$

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